



**HAL**  
open science

## Chromatic PAC-Bayes Bounds for Non-IID Data

Liva Ralaivola, Marie Szafranski, Guillaume Stempfel

► **To cite this version:**

Liva Ralaivola, Marie Szafranski, Guillaume Stempfel. Chromatic PAC-Bayes Bounds for Non-IID Data. 2008. hal-00336147v1

**HAL Id: hal-00336147**

**<https://hal.science/hal-00336147v1>**

Preprint submitted on 3 Nov 2008 (v1), last revised 10 Sep 2009 (v3)

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

---

# Chromatic PAC-Bayes Bounds for Non-IID Data

---

Liva Ralaivola, Marie Szafranski, Guillaume Stempfel

Laboratoire d'Informatique Fondamentale de Marseille

39, rue F. Joliot Curie, F-13013 Marseille, France

firstname.lastname@lif.univ-mrs.fr

## Abstract

PAC-Bayes bounds are among the most accurate generalization bounds for classifiers learned with IID data, and it is particularly so for margin classifiers. However, there are many practical cases where the training data show some dependencies and where the traditional IID assumption does not apply. Stating generalization bound for such frameworks is therefore of the utmost interest. In this work, we propose the first, to the best of our knowledge, PAC-Bayes generalization bound for classifiers trained on data exhibiting dependencies. The approach is based on the decomposition of a so-called dependency graph of the data in sets of independent data, through the tool of fractional covers. Our bounds are very general, since being able to find an upper bound on the chromatic number of the dependency graph is sufficient for it get new bounds for specific settings. We show how our results can be used to derive bounds for bipartite ranking and windowed prediction.

## 1 Introduction

Over the past decade there has been much progress in the field of generalization bounds for classifiers. Among the most appealing advances are the framework of PAC-Bayes bounds, first introduced by McAllester (1999), and later refined in several occasions (see (Seeger, 2002; Langford, 2005)). Their possible tightness, as witnessed by the work of Ambroladze et al. (2007), make them a possible route to perform model selection. They can also be viewed as theoretical tools to build new learning procedures.

Unfortunately, up to now, such bounds only hold for the case of classifiers trained from IID data, while being able to deal with non-IID data is a problem that can show up for real world applications such as, for instance,  $k$ -partite

ranking problem and windowed prediction. In this paper, we propose the first PAC-Bayes bounds for non-IID data; they are a direct generalization of the standard PAC-Bayes bound and they are general enough to provide a principled way to establish generalization bounds for a number of non-IID settings. To derive these new bounds, we will only make use of standard and very simple tools of probability theory and convexity properties of adequate functions, while exploiting the notion of fractional covers of graphs. This tool from graph theory has already been used for deriving concentration results for non independent data by Janson (2004) (see also references of work making use of such decompositions therein) and for providing generalization bound based on the so-called fractional Rademacher complexity by Usunier et al. (2006).

The paper is organized as follows. Section 2 first recall the standard IID Pac-Bayes bound, introduces the notion of fractional covers of graphs and then states the new *chromatic* PAC-Bayes bounds (called so, because they rely on the fractional chromatic number of a particular graph, namely the dependency graph of the data at hand). Section 3 is devoted to the proof of our main theorem. In Section 4, we provide specific versions of one of our bounds for the case of IID data, showing that it is a direct generalization of the standard bounds, and for the case of bipartite ranking and windowed prediction.

## 2 PAC Bayes Bounds based on Fractional Covers

### 2.1 IID PAC-Bayes Bound

Let us introduce some notation that will hold from here on. We only consider the problem of binary classification over the *input space*  $\mathcal{X}$  and we denote  $\mathcal{Z}$  the product space  $\mathcal{X} \times \mathcal{Y}$ , with  $\mathcal{Y} = \{-1, +1\}$ .  $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$  is a family of classifiers from  $\mathcal{X}$ .  $D$  is a probability distribution defined on  $\mathcal{Z}$  and  $\mathbf{D}_m$  the distribution of an  $m$ -sample; for instance,  $\mathbf{D}_m = \otimes_{i=1}^m D = D^m$  is the distribution of an IID sample  $\mathbf{Z} = \{Z_i\}_{i=1}^m$  of size  $m$ , with each  $Z_i$  distributed according

to  $D$ .  $P$  and  $Q$  are distributions over  $\mathcal{H}$ .

The usual PAC-Bayes bound, as first introduced by McAllester (1999) and later refined by Seeger (2002), can be stated as follows.

**Theorem 1** (IID PAC-Bayes Bound).  $\forall m, \forall D, \forall \mathcal{H}, \forall \delta \in (0, 1], \forall P$ , with probability at least  $1 - \delta$  over the random draw of  $\mathbf{Z} \sim \mathbf{D}_m$ , the following holds:

$$\forall Q, \text{kl}(\hat{e}_Q \| e_Q) \leq \frac{1}{m} \left[ \text{KL}(Q \| P) + \ln \frac{m+1}{\delta} \right]. \quad (1)$$

This theorem actually provides a generalization error bound for the so-called Gibbs classifier  $g_Q$ : given a distribution  $Q$  over  $\mathcal{H}$ , this stochastic classifier predicts a class for an input  $\mathbf{x} \in \mathcal{X}$  by first drawing a hypothesis  $h$  according to  $Q$  and then outputting  $h(\mathbf{x})$ . In the theorem,  $\hat{e}_Q$  is the empirical error of  $g_Q$  on an IID sample  $\mathbf{Z}$  of size  $m$  and  $e_Q$  is its true error:

$$\begin{aligned} \hat{e}_Q &= \mathbb{E}_{h \sim Q} \frac{1}{m} \sum_{i=1}^m r(h, Z_i) = \mathbb{E}_{h \sim Q} \hat{R}(h, \mathbf{Z}) \\ e_Q &= \mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \hat{e}_Q = \mathbb{E}_{\substack{Z \sim D \\ h \sim Q}} r(h, Z) = \mathbb{E}_{h \sim Q} R(h), \end{aligned} \quad (2)$$

where, for  $Z = (X, Y)$ ,  $r(h, Z) = \mathbb{I}_{h(X) \neq Y}$  and where we have used the fact that  $\mathbf{Z}$  is an (independently) identically distributed sample.  $\text{kl}(q \| p)$  is the Kullback-Leibler divergence between the Bernoulli distributions with probabilities of success  $q$  and  $p$ , and  $\text{KL}(Q \| P)$  is the Kullback-Leibler divergence between  $Q$  and  $P$ :

$$\begin{aligned} \text{kl}(q \| p) &= q \ln \frac{q}{p} + (1-q) \ln \frac{1-q}{1-p} \\ \text{KL}(Q \| P) &= \mathbb{E}_{h \sim Q} \ln \frac{Q(h)}{P(h)}. \end{aligned}$$

Throughout the paper, we make the assumption that the posteriors that are used are absolutely continuous with respect to their corresponding priors.

The problem we are interested in in the present work is that of generalizing Theorem 1 to the situation where there may exist probabilistic dependencies between the elements  $Z_i$  of  $\mathbf{Z} = \{Z_i\}_{i=1}^m$  but while, at the same time, the marginal distributions of the  $Z_i$ 's are identical. In other words, we provide PAC-Bayes bounds for classifiers trained on identically distributed data. These results rely on properties of a dependency graph that is built according to the dependencies within  $\mathbf{Z}$ . Before stating our new bounds, we thus introduce the concepts of graph theory that will play a role in their statements.

## 2.2 Dependency Graphs and Fractional Covers

**Definition 1** (Dependency Graph). Let  $\mathbf{Z} = \{Z_i\}_{i=1}^m$  be a set of random variables taking values in some space  $\mathcal{Z}$ . The *dependency graph*  $\Gamma(\mathbf{Z})$  of  $\mathbf{Z}$  is such that: the set of

vertices of  $\Gamma(\mathbf{Z})$  is  $\{1, \dots, m\}$  and there is an edge between  $i$  and  $j$  if and only if  $Z_i$  and  $Z_j$  are not independent (in the probabilistic sense).

**Definition 2** (Fractional Covers, see, e.g. Schreinerman and Ullman (1997)). Let  $\Gamma = (V, E)$  be an undirected graph, with  $V = \{1, \dots, m\}$ .

- $C \subseteq V$  is *independent* if the vertices in  $C$  are independent (in the graph theory sense: no two vertices in  $C$  are connected).
- $\mathbf{C} = \{C_j\}_{j=1}^n$ , with  $C_j \subseteq V$ , is a *proper cover* of  $V$  if each  $C_j$  is independent and  $\bigcup_{j=1}^n C_j = V$ . The size of  $\mathbf{C}$  is  $n$ .
- $\mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n$ , with  $C_j \subseteq V$  and  $\omega_j \in [0, 1]$ , is a *proper exact fractional cover* of  $V$  if each  $C_j$  is independent and  $\forall i \in V, \sum_{j=1}^n \omega_j \mathbb{I}_{i \in C_j} = 1$ ;  $\omega(\mathbf{C}) = \sum_{j=1}^n \omega_j$  is the *chromatic weight* of  $\mathbf{C}$ .
- $\chi(\Gamma)$  is the size of the smallest exact proper cover(s) of  $\Gamma$ : it is the *chromatic number* of  $\Gamma$ .
- $\chi^*(\Gamma)$  is the minimum weight over all proper exact fractional cover of  $V$ : it is the *fractional chromatic number* of  $\Gamma$ .

The problem of computing the (fractional) chromatic number of a graph is known to be NP-hard (Schreinerman & Ullman, 1997). However, it turns out that for some particular graphs as those that come from the settings we study in section 4, this number can be evaluated precisely. We, in particular have the following properties.

**Property 1** (Schreinerman and Ullman (1997)). Let  $\Gamma = (V, E)$  be a graph. Let  $c(\Gamma)$  be the clique number of  $\Gamma$ , i.e. the order of the largest clique in  $\Gamma$ . Let  $\Delta(\Gamma)$  be the maximum degree of a vertex in  $\Gamma$ .

We have the following inequalities:

$$1 \leq c(\Gamma) \leq \chi^*(\Gamma) \leq \chi(\Gamma) \leq \Delta(\Gamma) + 1.$$

In addition,  $1 = c(\Gamma) = \chi^*(\Gamma) = \chi(\Gamma) = \Delta(\Gamma) + 1$  if and only if  $\Gamma$  is *totally disconnected*.

*Remark 1.* A cover can be thought of a fractional cover with every  $w_i$  being equal to 1. Therefore, all the results that we state for fractional covers directly apply to the case of covers.

*Remark 2.* If  $\mathbf{Z} = \{Z_i\}_{i=1}^m$  is a set of random variables over  $\mathcal{Z}$  then a (fractional) proper cover of  $\Gamma(\mathbf{Z})$ , splits  $\mathbf{Z}$  into subsets of independent random variables. This is a crucial feature to establish the results of the present paper.

The following lemma, also taken from Janson (2004), Lemma 3.1, will be very useful in the following.

**Lemma 1.** If  $\mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^m$  is an exact fractional cover of  $\Gamma$  then

$$\forall \mathbf{t} \in \mathbb{R}^m, \sum_{i=1}^m t_i = \sum_{j=1}^n \omega_j \sum_{k \in C_j} t_k.$$

In particular  $m = \sum_{j=1}^n |C_j|$ .

### 2.3 Chromatic PAC-Bayes Bounds

In this subsection, we provide new PAC-Bayes bounds that apply for classifiers trained from samples  $\mathbf{Z}$  according to distributions  $\mathbf{D}_m$  where dependencies exist. Note that those dependencies are fully determined by  $\mathbf{D}_m$  and we can define the dependency graph  $\Gamma(\mathbf{D}_m)$  of  $\mathbf{D}_m$  to be  $\Gamma(\mathbf{D}_m) = \Gamma(\mathbf{Z})$ . As stated before, we make the assumption that the marginal distributions of  $\mathbf{D}_m$  along each coordinate are equal to  $D$ .

In the following theorems (and corresponding proofs) the following additional notation is considered.  $\text{PEFC}(\mathbf{D}_m)$  is the set of proper exact fractional covers of  $\Gamma(\mathbf{D}_m)$ . Given a cover  $\mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n \in \text{PEFC}(\mathbf{D}_m)$ ,  $\mathbf{Z}^{(j)} = \{Z_k\}_{k \in C_j}$  and  $\mathbf{D}_m^{(j)}$  is the distribution of  $\mathbf{Z}^{(j)}$ , it is therefore equal to  $D^{|C_j|}$ ;  $\alpha \in \mathbb{R}^n$  is the vector of coefficients  $\alpha_j = \omega_j / \omega(\mathbf{C})$  and  $\pi \in \mathbb{R}^n$  is the vector of coefficients  $\pi_j = \omega_j |C_j| / m$ .  $\mathbf{P}_n$  and  $\mathbf{Q}_n$  are distributions over  $\mathcal{H}^n$ ,  $P_n^j$  and  $Q_n^j$  are the marginal distributions of  $\mathbf{P}_n$  and  $\mathbf{Q}_n$  with respect to the  $j$ th coordinate, respectively;  $\mathbf{h} = (h_1, \dots, h_n)$  denotes a vector of  $n$  hypotheses from  $\mathcal{H}$ .

**Theorem 2** (Chromatic PAC-Bayes Bound (I)).  $\forall m, \forall \mathbf{D}_m, \forall \mathcal{H}, \forall \delta \in (0, 1], \forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n \in \text{PEFC}(\mathbf{D}_m), \forall \mathbf{P}_n$ , with probability at least  $1 - \delta$  over the random drawn of  $\mathbf{Z} \sim \mathbf{D}_m$ , the following holds:

$$\forall \mathbf{Q}_n, kl(\bar{e}_{\mathbf{Q}_n} | e_{\mathbf{Q}_n}) \leq \frac{\omega}{m} \left[ \sum_{j=1}^n \alpha_j KL(Q_n^j || P_n^j) + \ln \frac{m + \omega}{\delta \omega} \right], \quad (3)$$

where  $\omega$  stands for  $\omega(\mathbf{C})$  and

$$\begin{aligned} \bar{e}_{\mathbf{Q}_n} &= \mathbb{E}_{\mathbf{h} \sim \mathbf{Q}_n} \frac{1}{m} \sum_{j=1}^n \omega_j \sum_{k \in C_j} r(h_j, Z_k) \\ &= \frac{1}{m} \sum_{j=1}^n \omega_j |C_j| \mathbb{E}_{h \sim Q_n^j} \frac{1}{|C_j|} \sum_{k \in C_j} r(h, Z_k) \\ &= \sum_{j=1}^n \pi_j \mathbb{E}_{h \sim Q_n^j} \hat{R}(h, \mathbf{Z}^{(j)}). \end{aligned}$$

As usual,  $e_{\mathbf{Q}_n} = \mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \bar{e}_{\mathbf{Q}_n}$ .

The proof of this theorem is deferred to Section 3.

*Remark 3.* The empirical error  $\bar{e}_{\mathbf{Q}_n}$  considered in this theorem is a weighted average of the empirical errors on  $\mathbf{Z}^{(j)}$  of Gibbs classifiers with respective distributions  $Q_n^j$ .

The following proposition characterizes  $\mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \bar{e}_{\mathbf{Q}_n}$ .

**Proposition 1.**  $\forall m, \forall \mathbf{D}_m, \forall \mathcal{H}, \forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n \in \text{PEFC}(\mathbf{D}_m), \forall \mathbf{Q}_n$ ,  $e_{\mathbf{Q}_n} = \mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \bar{e}_{\mathbf{Q}_n}$  is the error of the Gibbs classifier based on the mixture of distributions  $Q^\pi = \sum_{j=1}^n \pi_j Q_n^j$  over  $\mathcal{H}$ .

*Proof.* From Definition 2,  $\pi_j \geq 0$  and, according to Lemma 1,  $\sum_{j=1}^n \pi_j = \frac{1}{m} \sum_{j=1}^n \omega_j |C_j| = 1$ .

Then,

$$\begin{aligned} \mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \bar{e}_{\mathbf{Q}_n} &= \sum_j \pi_j \mathbb{E}_{h \sim Q_j} \mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \hat{R}(h, \mathbf{Z}^{(j)}) \\ &= \sum_j \pi_j \mathbb{E}_{h \sim Q_j} \mathbb{E}_{\mathbf{Z}^{(j)} \sim \mathbf{D}_m^{(j)}} \hat{R}(h, \mathbf{Z}^{(j)}) \\ &= \sum_j \pi_j \mathbb{E}_{h \sim Q_n^j} R(h) \\ &= \mathbb{E}_{h \sim \pi_1 Q_n^1 + \dots + \pi_n Q_n^n} R(h) = \mathbb{E}_{h \sim Q^\pi} R(h). \end{aligned}$$

□

Noting that the prior  $\mathbf{P}_n$  and the posterior  $\mathbf{Q}_n$  enter into play in this proposition and Theorem 2 through their marginals only, these results advocate for the following learning scheme. Given a cover and a (possibly factorized) prior  $\mathbf{P}_n$ , look for a factorized posterior  $\mathbf{Q}_n = \otimes_{j=1}^n Q_j$  such that each  $Q_j$  independently minimizes the usual IID PAC-Bayes bound given in Theorem 1 on each  $\mathbf{Z}^{(j)}$ . Then make predictions according to the Gibbs classifier defined with respect to  $Q^\pi = \sum_j \pi_j Q_j$ .

The following theorem gives a result that can be readily used without choosing a specific cover.

**Theorem 3** (Chromatic PAC-Bayes Bound (II)).  $\forall m, \forall \mathbf{D}_m, \forall \mathcal{H}, \forall \delta \in (0, 1], \forall P$ , with probability at least  $1 - \delta$  over the random draw of  $\mathbf{Z} \sim \mathbf{D}_m$ , the following holds

$$\forall Q, kl(\hat{e}_Q | e_Q) \leq \frac{\chi^*}{m} \left[ KL(Q || P) + \ln \frac{m + \chi^*}{\delta \chi^*} \right], \quad (4)$$

where  $\chi^*$  is the fractional chromatic number of  $\Gamma(\mathbf{D}_m)$ , and where  $\hat{e}_Q$  and  $e_Q$  are defined as in (2).

*Proof.* This theorem is just a particular case of Theorem 2. Let us assume that  $\mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n \in \text{PEFC}(\mathbf{D}_m)$  such that  $\omega(\mathbf{C}) = \chi^*(\Gamma(\mathbf{D}_m))$ ,  $\mathbf{P}_n = \otimes_{j=1}^n P = P^n$  and  $\mathbf{Q}_n = \otimes_{j=1}^n Q = Q^n$ , with  $P$  and  $Q$  distributions over  $\mathcal{H}$ .

For the right-hand side (4), it directly comes that

$$\sum_j \alpha_j KL(Q_n^j || P_n^j) = \sum_j \alpha_j KL(Q || P) = KL(Q || P).$$

As for the left-hand side of (4), it suffices to show that

$\bar{e}_{\mathbf{Q}_n} = \hat{e}_Q$ :

$$\begin{aligned}
\bar{e}_{\mathbf{Q}_n} &= \sum_j \pi_j \mathbb{E}_{h \sim Q_n^j} \hat{R}(h, \mathbf{Z}^{(j)}) \\
&= \sum_j \pi_j \mathbb{E}_{h \sim Q} \hat{R}(h, \mathbf{Z}^{(j)}) \\
&= \frac{1}{m} \sum_j \omega_j |C_j| \mathbb{E}_{h \sim Q} \frac{1}{|C_j|} \sum_k r(h, Z_k) \\
&= \mathbb{E}_{h \sim Q} \frac{1}{m} \sum_j \omega_j \sum_k r(h, Z_k) \\
&= \mathbb{E}_{h \sim Q} \frac{1}{m} \sum_i r(h, Z_i) = \mathbb{E}_{h \sim Q} \hat{R}(h, \mathbf{Z}) = \hat{e}_Q.
\end{aligned}$$

□

*Remark 4.* This theorem says that even in the case of non IID data, a PAC-Bayes bound very similar to the IID PAC-Bayes bound (1) can be stated, with a worsening (since  $\chi^* \geq 1$ ) proportional to  $\chi^*$ , i.e proportional to the amount of dependencies that exist in the data under consideration. In addition, the new PAC-Bayes bounds is valid with any priors and posteriors, without the need for these distributions nor their marginals to depend on the structure of the dependency graph, or, in other words, on the chosen cover (as is the case in the more general Theorem 2 and the entailed algorithm).

*Remark 5.* We note that among all elements of PEFC( $\mathbf{D}_m$ ),  $\chi^*$  is the best constant achievable in terms of the tightness of the bound. Indeed, the function  $f_{m,\delta}(\omega) = \omega \ln \frac{m+\omega}{\delta\omega}$  is nondecreasing for all  $m \in \mathbb{N}$  and  $\delta \in (0, 1]$ , as indicated by the sign of the derivative  $f'_{m,\delta}$ :

$$\begin{aligned}
f'_{m,\delta}(\omega) &= -\ln \frac{\delta\omega}{m+\omega} + \frac{\omega}{m+\omega} - 1 \\
&\geq -\ln \frac{\omega}{m+\omega} + \frac{\omega}{m+\omega} - 1 \\
&\geq -\frac{\omega}{m+\omega} + 1 + \frac{\omega}{m+\omega} - 1 = 0
\end{aligned}$$

where we have used the well-known inequality  $\ln x \leq x - 1$ . Since  $\chi^*$  is the smallest chromatic weight, this actually is the weight that gives the tightest bound.

### 3 Proof of Theorem 2

A proof in three steps, following the lines of the proofs given by Seeger (2002) and Langford (2005) for the IID PAC-Bayes bound, can be provided for Theorem 2.

**Lemma 2.**  $\forall m, \forall \mathbf{D}_m, \forall \delta \in (0, 1], \forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n, \forall \mathbf{P}_n$ , with probability at least  $1 - \delta$  over the random draw of  $\mathbf{Z} \sim \mathbf{D}_m$ , the following holds

$$\mathbb{E}_{\mathbf{h} \sim \mathbf{P}_n} \sum_{j=1}^n \alpha_j e^{|C_j| \text{kl}(\hat{R}(h_j, \mathbf{Z}^{(j)}) || R(h_j))} \leq \frac{m + \omega}{\delta \omega}, \quad (5)$$

where  $\omega$  stands for  $\omega(\mathbf{C})$ .

*Proof.* We first observe the following:

$$\begin{aligned}
&\mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \sum_j \alpha_j e^{|C_j| \text{kl}(\hat{R}(h_j, \mathbf{Z}^{(j)}) || R(h_j))} \\
&= \sum_j \alpha_j \mathbb{E}_{\mathbf{Z}^{(j)} \sim \mathbf{D}_m^{(j)}} e^{|C_j| \text{kl}(\hat{R}(h, \mathbf{Z}^{(j)}) || R(h))} \\
&\leq \sum_j \alpha_j (|C_j| + 1) \quad (\text{cf. Theorem 5}) \\
&= \frac{1}{\omega} \sum_j \omega_j (|C_j| + 1) = \frac{m + \omega}{\omega},
\end{aligned}$$

where using Theorem 5 is made possible by the fact that  $\mathbf{Z}^{(j)}$  are IID Therefore,

$$\mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} \mathbb{E}_{\mathbf{h} \sim \mathbf{P}_n} \sum_{j=1}^n \alpha_j e^{|C_j| \text{kl}(\hat{R}(h_j, \mathbf{Z}^{(j)}) || R(h_j))} \leq \frac{m + \omega}{\omega}.$$

Applying Markov's inequality (cf. Theorem 7 in Appendix) to the random variable  $\mathbb{E}_{\mathbf{h} \sim \mathbf{P}_n} \sum_j \alpha_j e^{|C_j| \text{kl}(\hat{R}(h_j, \mathbf{Z}^{(j)}) || R(h_j))}$  gives the desired result. □

**Lemma 3.**  $\forall m, \forall \mathbf{D}_m, \forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n, \forall \mathbf{P}_n, \forall \mathbf{Q}_n$ , with probability at least  $1 - \delta$  over the random draw of  $\mathbf{Z} \sim \mathbf{D}_m$ , the following holds

$$\begin{aligned}
\frac{m}{\omega} \sum_{j=1}^n \pi_j \mathbb{E}_{h \sim Q_n^j} \text{kl}(\hat{R}(h, \mathbf{Z}^{(j)}) || R(h)) & \quad (6) \\
\leq \sum_{j=1}^n \alpha_j \text{KL}(Q_n^j || P_n^j) + \ln \frac{m + \omega}{\delta \omega}.
\end{aligned}$$

*Proof.* It suffices to use Jensen's inequality with  $\ln$  and the fact that  $\mathbb{E}_{X \sim P} f(X) = \mathbb{E}_{X \sim Q} \frac{P(X)}{Q(X)} f(X)$ , for all  $f, P, Q$ . Therefore,  $\forall \mathbf{Q}_n$ :

$$\begin{aligned}
&\ln \mathbb{E}_{\mathbf{h} \sim \mathbf{P}_n} \sum_j \alpha_j e^{|C_j| \text{kl}(\hat{R}(h_j, \mathbf{Z}^{(j)}) || R(h_j))} \\
&= \ln \sum_j \alpha_j \mathbb{E}_{h \sim P_n^j} e^{|C_j| \text{kl}(\hat{R}(h, \mathbf{Z}^{(j)}) || R(h))} \\
&= \ln \sum_j \alpha_j \mathbb{E}_{h \sim Q_n^j} \frac{P_n^j(h)}{Q_n^j(h)} e^{|C_j| \text{kl}(\hat{R}(h, \mathbf{Z}^{(j)}) || R(h))} \\
&\geq \sum_j \alpha_j \mathbb{E}_{h \sim Q_n^j} \ln \left[ \frac{P_n^j(h)}{Q_n^j(h)} e^{|C_j| \text{kl}(\hat{R}(h, \mathbf{Z}^{(j)}) || R(h))} \right] \\
&= - \sum_j \alpha_j \text{KL}(Q_n^j || P_n^j) \\
&\quad + \sum_j \alpha_j |C_j| \mathbb{E}_{h \sim Q_n^j} \text{kl}(\hat{R}(h, \mathbf{Z}^{(j)}) || R(h)) \\
&= - \sum_j \alpha_j \text{KL}(Q_n^j || P_n^j) \\
&\quad + \frac{m}{\omega} \sum_j \pi_j \mathbb{E}_{h \sim Q_n^j} \text{kl}(\hat{R}(h, \mathbf{Z}^{(j)}) || R(h)).
\end{aligned}$$

Lemma 2 then gives the result. □

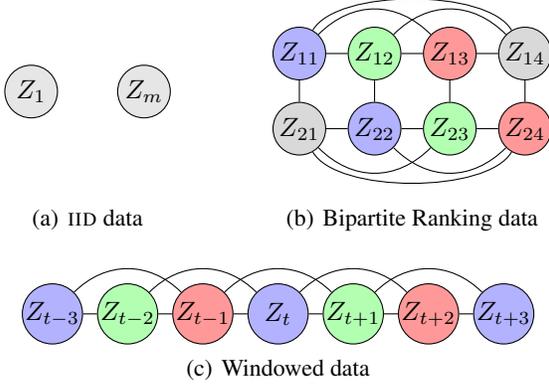


Figure 1: Dependency graphs for the different settings described in section 4: (a) when the data are IID, the dependency graph is disconnected and the fractional number is  $\chi^* = 1$ ; (b) a dependency graph obtained for bipartite ranking from a sample containing 4 positive instances and 2 negative instances; nodes of the same color are independent and  $\chi^* = 4$ ; (c) a dependency graph obtained with windowed prediction for a window parameter  $r = 1$  (see text for details):  $\chi^* = 2r + 1$ .

**Lemma 4.**  $\forall m, \forall \mathbf{D}_m, \forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n, \forall \mathbf{Q}_n$ , the following holds

$$\frac{m}{\omega} \sum_{j=1}^n \pi_j \mathbb{E}_{h \sim \mathcal{Q}_n^j} kl(\hat{R}(h, \mathbf{Z}^{(j)}) || R(h)) \geq kl(\bar{e}_Q || e_Q).$$

*Proof.* This simply comes from the application of Theorem 6. This lemma, in combination with Lemma 3, closes the proof of Theorem 2.  $\square$

## 4 Examples

In this section, we give instances of the bound given in Theorem 3 for different settings.

### 4.1 IID case

In the IID case, the training sample is  $\mathbf{Z} = \{(X_i, Y_i)\}_{i=1}^m$  distributed according to  $\mathbf{D}_m = D^m$  and the fractional chromatic number of  $\Gamma(\mathbf{D}_m)$  is  $\chi^* = 1$ . Plugging in this value of  $\chi^*$  in the bound of Theorem 3 gives the usual PAC-Bayes bound recalled in Theorem 1. This emphasizes that our results are generalizations of the standard PAC-Bayes bound.

### 4.2 Bipartite Ranking

Let  $\bar{D}$  be a distribution over  $\bar{\mathcal{X}} \times \bar{\mathcal{Y}}$  and  $\bar{D}_{+1}$  ( $\bar{D}_{-1}$ ) be the class conditional distribution  $\bar{D}_{X|Y=+1}$  ( $\bar{D}_{X|Y=-1}$ ) with respect to  $\bar{D}$ . In the bipartite ranking problem (see, e.g. (Agarwal et al., 2005)), one tries to control the misranking

risk, defined for  $f \in \mathbb{R}^{\mathcal{X}}$  by

$$R^{\text{rank}}(f) = \mathbb{P}_{\substack{\bar{X}^+ \sim \bar{D}_{+1} \\ \bar{X}^- \sim \bar{D}_{-1}}} (f(\bar{X}^+) \leq f(\bar{X}^-)). \quad (7)$$

$f$  can be interpreted as a scoring function. Given an IID sample  $\mathbf{S} = \{(\bar{X}_i, \bar{Y}_i)\}_{i=1}^\ell$  distributed according to  $\bar{D}_\ell = \bar{D}^\ell$ , a usual strategy to minimize (7) is to minimize (a possibly regularized form of)

$$\hat{R}^{\text{rank}}(f, \mathbf{S}) = \frac{1}{\ell^+ \ell^-} \sum_{\substack{i: \bar{Y}_i = +1 \\ j: \bar{Y}_j = -1}} r(f, (\bar{X}_i, \bar{X}_j)), \quad (8)$$

where  $r(f, (\bar{X}_i, \bar{X}_j)) = \mathbb{I}_{f(\bar{X}_i) \leq f(\bar{X}_j)}$  and  $\ell^+$  ( $\ell^-$ ) is the number of positive (negative) data in  $\mathbf{S}$ . This empirical risk, which is closely related to the AUC<sup>1</sup> (see (Agarwal et al., 2005; Cortes & Mohri, 2004)), estimates the fraction of pairs  $(\bar{X}_i, \bar{X}_j)$  that are ranked incorrectly (given that  $\bar{Y}_i = +1$  and  $\bar{Y}_j = -1$ ) and is an unbiased estimator of  $R^{\text{rank}}(h)$ . The entailed problem can be seen as that of learning a classifier from a training set of the form  $\mathbf{Z} = \{Z_{ij}\}_{ij} = \{(X_{ij} = (\bar{X}_i, \bar{X}_j), 1)\}_{ij}$ . This reveals the non-IID nature of the training data as  $Z_{ij}$  depends on  $\{Z_{pq} : p = i \text{ or } q = j\}$  (see Figure 1).

Using Theorem 3, we have the following result:

**Theorem 4.**  $\forall \ell, \forall \bar{D}$  over  $\bar{\mathcal{X}} \times \bar{\mathcal{Y}}, \forall \bar{\mathcal{H}} \subseteq \mathbb{R}^{\bar{\mathcal{X}}}, \forall \delta \in (0, 1], \forall \bar{P}$  over  $\bar{\mathcal{H}}$ , with probability at least  $1 - \delta$  over the random draw of  $\mathbf{S} \sim \bar{D}^\ell$ , the following holds

$$\forall \bar{Q} \text{ over } \bar{\mathcal{H}}, kl(\hat{e}_Q^{\text{rank}} || e_Q^{\text{rank}}) \leq \frac{1}{\ell_{\min}} \left[ KL(\bar{Q} || \bar{P}) + \ln \frac{\ell_{\min} + 1}{\delta} \right], \quad (9)$$

where  $\ell_{\min} = \min(\ell^+, \ell^-)$ , and  $\hat{e}_Q^{\text{rank}}$  and  $e_Q^{\text{rank}}$  are the Gibbs ranking error counterparts of (2) based on (7) and (8), respectively.

*Proof.* The proof works in three parts and borrows ideas from Agarwal et al. (2005).

**Conditioning on  $\mathbf{Y} = \mathbf{y}$ .** Let  $\mathbf{y} \in \{-1, +1\}^\ell$  be a fixed vector and  $\ell_{\mathbf{y}}^+$  and  $\ell_{\mathbf{y}}^-$  the number of positive and negative labels, respectively. We define the distribution  $\bar{D}_{\mathbf{y}}$  as  $\bar{D}_{\mathbf{y}} = \otimes_{i=1}^\ell \bar{D}_{y_i}$ ; this is a distribution on  $\bar{\mathcal{X}}^\ell$ . With a slight abuse of notation,  $\bar{D}_{\mathbf{y}}$  will also be used to denote the distribution over  $(\bar{\mathcal{X}} \times \bar{\mathcal{Y}})^\ell$  of samples  $\mathbf{S} = \{(\bar{X}_i, y_i)\}_{i=1}^\ell$  such that the sequence  $\{\bar{X}_i\}_{i=1}^\ell$  is distributed according to  $\bar{D}_{\mathbf{y}}$ . It is straightforward to check that,  $\forall f \in \bar{\mathcal{H}}, \mathbb{E}_{\mathbf{S} \sim \bar{D}_{\mathbf{y}}} \hat{R}^{\text{rank}}(f, \mathbf{S}) = \hat{R}^{\text{rank}}(f)$ .

Given  $\mathbf{S}$ , defining the random variable  $Z_{ij}$  as  $Z_{ij} = ((X_i, X_j), 1)$ ,  $\mathbf{Z} = \{Z_{ij}\}_{i: y_i=1, j: y_j=-1}$  is a sample of identically distributed variables, each with distribution  $D_{\pm 1} = \bar{D}_{+1} \otimes \bar{D}_{-1} \otimes \mathbf{1}$  over  $\mathcal{X} \times \mathcal{Y}$ , where  $\mathcal{X} = \bar{\mathcal{X}} \times \bar{\mathcal{X}}$ ,

<sup>1</sup>It is actually 1-AUC.

$\mathcal{Y} = \{-1, +1\}$  and  $\mathbf{1}$  is the distribution that produces 1 with probability 1.

If we let  $m = \ell_y^+ \ell_y^-$ , the training sample  $\mathbf{Z}$  is distributed according to  $\mathbf{D}_{\mathbf{y}, m} = \otimes_{i=1}^m D_{\pm 1} = D_{\pm 1}^m$ , where interdependencies exist, as shown on Figure 1. Theorem 2 can thus be directly applied to classifiers trained on  $\mathbf{Z}$ , the structure of  $\Gamma(\mathbf{D}_{\mathbf{y}, m})$  and its corresponding fractional chromatic number  $\chi_{\mathbf{y}}^*$  being completely determined by  $\mathbf{y}$ . Letting  $\mathcal{H} \subseteq \mathcal{Y}^{\mathcal{X}}$ ,  $\forall \delta \in (0, 1]$ ,  $\forall P$  over  $\mathcal{H}$ , with probability at least  $1 - \delta$  over the random draw of  $\mathbf{Z} \sim \mathbf{D}_{\mathbf{y}, m}$ ,

$$\forall Q \text{ over } \mathcal{H}, \text{kl}(\hat{e}_Q \| e_Q) \leq \frac{\chi_{\mathbf{y}}^*}{m} \left[ \text{KL}(Q \| P) + \ln \frac{m + \chi_{\mathbf{y}}^*}{\delta \chi_{\mathbf{y}}^*} \right].$$

Given  $f \in \overline{\mathcal{H}}$ , it is straightforward to see that for  $h_f \in \mathcal{Y}^{\mathcal{X}}$  defined as  $h_f((X, X')) = \text{sign}(f(X) - f(X'))$ , with  $\text{sign}(x) = +1$  if  $x > 0$  and  $-1$  otherwise,  $\hat{R}(h_f, \mathbf{Z}) = \hat{R}^{\text{rank}}(f, \mathbf{S})$  and  $\mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_{\mathbf{y}, m}} \hat{R}(h_f, \mathbf{Z}) = \mathbb{E}_{\mathbf{S} \sim \overline{\mathbf{D}}_{\mathbf{y}}} \hat{R}^{\text{rank}}(f, \mathbf{S}) = R^{\text{rank}}(f)$ . Hence,  $\forall \delta \in (0, 1]$ ,  $\forall \overline{P}$  over  $\overline{\mathcal{H}}$ , with probability at least  $1 - \delta$  over the random draw of  $\mathbf{S} \sim \overline{\mathbf{D}}_{\mathbf{y}}$ ,

$$\forall \overline{Q}, \text{kl}(\hat{e}_{\overline{Q}}^{\text{rank}} \| e_{\overline{Q}}^{\text{rank}}) \leq \frac{\chi_{\mathbf{y}}^*}{m} \left[ \text{KL}(\overline{Q} \| \overline{P}) + \ln \frac{m + \chi_{\mathbf{y}}^*}{\delta \chi_{\mathbf{y}}^*} \right]. \quad (10)$$

**Integrating over  $\mathbf{Y}$ .** As proposed by Agarwal et al. (2005), let us call  $\Phi(\overline{P}, \mathbf{S}, \delta)$  the event (10); we just stated that  $\forall \mathbf{y} \in \{-1, +1\}^{\ell}$ ,  $\forall \overline{P}, \forall \delta \in (0, 1]$ ,  $\mathbb{P}_{\mathbf{S} \sim \overline{\mathbf{D}}_{\mathbf{y}}}(\Phi(\overline{P}, \mathbf{S}, \delta)) \geq 1 - \delta$ . Then,  $\forall \overline{P}, \forall \delta \in (0, 1]$ ,

$$\begin{aligned} \mathbb{P}_{\mathbf{S} \sim \overline{\mathbf{D}}_{\ell}}(\Phi(\overline{P}, \mathbf{S}, \delta)) &= \mathbb{E}_{\mathbf{Y}}[\mathbb{E}_{\mathbf{S} \sim \mathbf{D}_{\mathbf{Y}}} \mathbb{I}_{\Phi(\overline{P}, \mathbf{S}, \delta)}] \\ &= \sum_{\mathbf{y}} \mathbb{E}_{\mathbf{S} \sim \overline{\mathbf{D}}_{\mathbf{y}}} \mathbb{I}_{\Phi(\overline{P}, \mathbf{S}, \delta)} \mathbb{P}(\mathbf{Y} = \mathbf{y}) \\ &= \sum_{\mathbf{y}} \mathbb{P}_{\mathbf{S} \sim \overline{\mathbf{D}}_{\mathbf{y}}}(\Phi(\overline{P}, \mathbf{S}, \delta)) \mathbb{P}(\mathbf{Y} = \mathbf{y}) \\ &\geq \sum_{\mathbf{y}} (1 - \delta) \mathbb{P}(\mathbf{Y} = \mathbf{y}) = 1 - \delta. \end{aligned}$$

Hence,  $\forall \delta \in (0, 1]$ ,  $\forall \overline{P}$  over  $\overline{\mathcal{H}}$ , with probability at least  $1 - \delta$  over the random draw of  $\mathbf{S} \sim \overline{\mathbf{D}}_{\ell}$ ,

$$\forall \overline{Q}, \text{kl}(\hat{e}_{\overline{Q}}^{\text{rank}} \| e_{\overline{Q}}^{\text{rank}}) \leq \frac{\chi_{\mathbf{S}}^*}{m_{\mathbf{S}}} \left[ \text{KL}(\overline{Q} \| \overline{P}) + \ln \frac{m_{\mathbf{S}} + \chi_{\mathbf{S}}^*}{\delta \chi_{\mathbf{S}}^*} \right]. \quad (11)$$

where  $\chi_{\mathbf{S}}^*$  is the fractional chromatic number of the graph  $\Gamma(\mathbf{Z})$ , with  $\mathbf{Z}$  defined from  $\mathbf{S}$  as in the first part of the proof (taking into account the observed labels in  $\mathbf{S}$ ); here  $m_{\mathbf{S}} = \ell^+ \ell^-$ , where  $\ell^+$  ( $\ell^-$ ) is the number of positive (negative) data in  $\mathbf{S}$ .

**Computing the Fractional Chromatic Number.** In order to finish the proof, it suffices to observe that, for  $\mathbf{Z} = \{Z_{ij}\}_{ij}$ , letting  $\ell_{\max} = \max(\ell^+, \ell^-)$ , the fractional chromatic number of  $\Gamma(\mathbf{Z})$  is  $\chi^* = \ell_{\max}$ .

Indeed, the clique number of  $\Gamma(\mathbf{Z})$  is  $\ell_{\max}$  as for all  $i = 1, \dots, \ell^+$  ( $j = 1, \dots, \ell^-$ ),  $\{Z_{ij} : j = 1, \dots, \ell^-\}$  ( $\{Z_{ij} : i = 1, \dots, \ell^+\}$ ) defines a clique of order  $\ell^-$  ( $\ell^+$ ) in  $\Gamma(\mathbf{Z})$ . Thus, from Property 1:  $\chi \geq \chi^* \geq \ell_{\max}$ .

A proper exact cover  $\mathbf{C} = \{C_k\}_{k=1}^{\ell_{\max}}$  of  $\Gamma(\mathbf{Z})$  can be constructed as follows<sup>2</sup>. Suppose that  $\ell_{\max} = \ell^+$ , then  $C_k = \{Z_{i\sigma_k(i)} : i = 1, \dots, \ell^-\}$ , with

$$\sigma_k(i) = (i + k - 2 \pmod{\ell^+}) + 1,$$

is an independent set: no two variables  $Z_{ij}$  and  $Z_{pq}$  in  $C_k$  are such that  $i = p$  or  $j = q$ . In addition, it is straightforward to check that  $\bigcup_{k=1}^{\ell^+} C_k$  is a cover of  $\Gamma(\mathbf{Z})$ . This cover is of size  $\ell^+ = \ell_{\max}$ , which means that it achieves the minimal possible weight over proper exact (fractional) covers since  $\chi^* \geq \ell_{\max}$ . Hence,  $\chi^* = \chi = \ell_{\max} (= c(\Gamma))$ . Plugging in this value of  $\chi^*$  in (11), and noting that  $m_{\mathbf{S}} = \ell_{\max} \ell_{\min}$  with  $\ell_{\min} = \min(\ell^+, \ell^-)$ , closes the proof.  $\square$

As proposed by Langford (2005) (section 5.3), the PAC-Bayes bound of Theorem 4 can be specialized to the case where  $\overline{\mathcal{H}} = \{f : f(x) = w \cdot x, w \in \overline{\mathcal{X}}\}$ . In this situation, for  $f \in \overline{\mathcal{H}}$ ,  $h_f((X, X')) = \text{sign}(f(X) - f(X')) = \text{sign}(w \cdot (X - X'))$  is simply a linear classifier (the argument carries over to the use of kernel classifiers). Hence, assuming an isotropic Gaussian prior  $P = \mathcal{N}(0, I)$  and a family of posteriors  $Q_{w, \mu}$  parameterized by  $w \in \overline{\mathcal{X}}$  and  $\mu > 0$  such that  $Q_{w, \mu}$  is  $\mathcal{N}(\mu, 1)$  in the direction  $w$  and  $\mathcal{N}(0, 1)$  in all perpendicular directions, we arrive at the following theorem (of which we do not provide the proof):

**Theorem 5.**  $\forall \ell, \forall \overline{D}$  over  $\overline{\mathcal{X}} \times \overline{\mathcal{Y}}$ ,  $\forall \delta \in (0, 1]$ , the following holds with probability at least  $1 - \delta$  over the draw of  $\mathbf{S} \sim \overline{D}^{\ell}$ :

$$\forall w, \mu > 0, \text{kl}(\hat{R}_{Q_{w, \mu}}^{\text{rank}} \| R_{Q_{w, \mu}}^{\text{rank}}) \leq \frac{1}{\ell_{\min}} \left[ \frac{\mu^2}{2} + \ln \frac{\ell_{\min} + 1}{\delta} \right].$$

The bounds given in Theorem 4 and Theorem 5 are very similar to what we would get if applying IID PAC-Bayes bound to one (independent) element  $C_j$  of a minimal cover (i.e. their weight equals the fractional chromatic number)  $\mathbf{C} = \{C_j\}_{j=1}^n$  such as the one we have constructed in the proof of Theorem 4. The main point is that it would imply the empirical error to be computed on a specific  $C_j$  and not on the whole data as is the case for the new results. It turns out that, for proper exact fractional covers  $\mathbf{C} = \{(C_j, \omega)\}_{j=1}^n$  with elements  $|C_j|$  having the same size, it is better, in terms of absolute moments of the empirical error, to assess it on the whole dataset, rather than on only one  $C_j$ . The following proposition formalizes this statement.

<sup>2</sup>Note that the cover defined here consider elements  $C_k$  containing random variables instead of indices of random variable as before. This abuse of notation is made for sake of readability.

**Proposition 2.**  $\forall m, \forall \mathbf{D}_m, \forall \mathcal{H}, \forall \mathbf{C} = \{(C_j, \omega_j)\}_{j=1}^n \in \text{PEFC}(\mathbf{D}_m), \forall Q, \forall r \in \mathbb{N}, r \geq 1,$

$$\mathbb{E}_{\mathbf{Z} \sim \mathbf{D}_m} |\hat{e}_Q - e_Q|^r \leq \mathbb{E}_{\mathbf{Z}^{(j)} \sim \mathbf{D}_m^{(j)}} |\hat{e}_Q - e_Q|^r,$$

where  $\mathbf{D}_m^{(j)}$  is the marginal distribution of  $\mathbf{Z}^{(j)}$ .

*Proof.* It suffices to use the convexity of  $|\cdot|^r$  for  $r \geq 1$  and the linearity of  $\mathbb{E}$ . Using notation of section 2, we have, for  $\mathbf{Z} \sim \mathbf{D}_m$ :

$$\begin{aligned} |\hat{e}_Q - e_Q|^r &= \left| \sum_j \pi_j \mathbb{E}_{h \sim Q} (\hat{R}(h, \mathbf{Z}^{(j)}) - R(h)) \right|^r \\ &\leq \sum_j \pi_j |\mathbb{E}_{h \sim Q} (\hat{R}(h, \mathbf{Z}^{(j)}) - R(h))|^r. \end{aligned}$$

Taking the expectation of both sides with respect to  $\mathbf{Z}$  and observing that all the  $\mathbf{Z}^{(j)}$ , and thus, all the random variables  $|\mathbb{E}_{h \sim Q} (\hat{R}(h, \mathbf{Z}^{(j)}) - R(h))|^r$ , have the same distribution gives the result.  $\square$

### 4.3 Predictions on Centered Windows

There are many situations, such as in bioinformatics, where a classifier must be learned from a training sample  $\mathbf{S} = \{(\bar{X}_t, \bar{Y}_t)\}_{t=1}^T \in (\bar{\mathcal{X}} \times \mathcal{Y})^T$  where it is known that, in order to predict  $\bar{Y}_t$ , information from a *window*  $\{\bar{X}_{t+\tau}\}_{\tau=-r}^r$  of  $2r + 1$  data centered on  $\bar{X}_t$  must be considered (such a scheme has been used for prediction of the secondary structure of proteins, for instance). This problem can be recast in another classification problem using a training sample  $\mathbf{Z} = \{Z_t\}_{t=1}^T$ , with  $Z_t = ((\bar{X}_{t-r}, \dots, \bar{X}_t, \dots, \bar{X}_{t+r}), \bar{Y}_t)$ , with special care taken for  $t \leq r + 1$  and  $t > T - r$ . Considering that  $\bar{\mathcal{Y}} = \{-1, +1\}$ , the input space and output space to be considered are therefore  $\mathcal{X} = \bar{\mathcal{X}}^{2r+1}$  and  $\mathcal{Y} = \bar{\mathcal{Y}}$ ; the product space is  $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$ . As for the bipartite ranking problem, we end up with a learning problem from non-IID data,  $\mathbf{Z}$  having a dependency graph  $\Gamma(\mathbf{Z})$  as the one depicted on Figure 1.

It is easy to see that the clique number of  $\Gamma(\mathbf{Z})$  is  $2r + 1$ . Besides, one can construct a proper exact cover  $\mathbf{C} = \{C_j\}_j$  of minimal weight by taking  $C_j = \{Z_{j+p(2r+1)} : p = 1, \dots, (T - (2r + 1))/j\}$ , for  $j = 1, \dots, 2r + 1$  – we make the implicit and reasonable assumption that  $T > 2r + 1$ . This cover is proper and has size  $2r + 1$ . Invoking Property 1 gives that  $\chi = \chi^* = 2r + 1$ .

It is therefore easy to get a new PAC-Bayes theorem for the case of windowed prediction, by replacing  $\chi^*$  by  $2r + 1$  and  $m$  by  $T$  in the bound (4) of Theorem 3. We do not state it explicitly for sake of conciseness.

## 5 Conclusion

In this work, we propose the first PAC-Bayes bounds for non-IID data. The derivation of these results rely on the

use of fractional covers of graphs, convexity and standard tools from probability theory. The results that we provide are very general and can easily be instantiated for specific learning settings such as bipartite ranking and windowed prediction.

This work gives rise to many interesting questions. First, it seems that using a fractional cover to decompose the non-IID training data into sets of IID data and then tightening the bound through the use of the chromatic number is some form of variational relaxation as often encountered in the context of making inference in graphical models. It might be interesting to make this connection clearer to see if, for instance, tighter bounds can be obtained with softer variational relaxations than the one incurred by the use of fractional covers.

Besides, Theorem 2 advocates for a particular learning algorithm, as noted previously. It would be interesting to see how such a learning algorithm could perform empirically and how tight the proposed bound could be. On another empirical side, we are currently running experiments on bipartite ranking problems to see how accurate the bound of Theorem 4 can be: the results are very encouraging.

Finally, it remains the question as to what kind of strategies to learn the prior(s) could be implemented to render the bounds that we get the tightest possible. This is one of the most stimulating question as performing such prior learning makes it possible to obtain very accurate generalization bound, as evidenced by the work of Ambroladze et al. (2007).

## Appendix

This appendix gathers useful results for the different proofs. Only sketches of their proofs or even just references are given.

**Lemma 5.** *Let  $D$  be a distribution over  $\mathcal{Z}$ .*

$$\forall h \in \mathcal{H}, \mathbb{E}_{\mathbf{Z} \sim D^m} e^{mkl(\hat{R}(h, \mathbf{Z}) || R(h))} \leq m + 1.$$

*Proof.* Let  $h \in \mathcal{H}$ . For  $\mathbf{z} \in \mathcal{Z}^m$ , we let  $q(\mathbf{z}) = \hat{R}(h, \mathbf{z})$ ; we also let  $p = R(h)$ . Note that since  $\mathbf{Z}$  is i.i.d,  $mQ(\mathbf{Z})$  is binomial with parameters  $m$  and  $p$  (recall that  $r(h, Z)$  takes the values 0 and 1 upon correct and erroneous classification

of  $Z$  by  $h$ , respectively).

$$\begin{aligned}
& \mathbb{E}_{\mathbf{Z} \sim D^m} e^{m \text{kl}(q(\mathbf{Z})||p)} \\
&= \sum_{\mathbf{z} \in \mathcal{Z}^m} e^{m \text{kl}(q(\mathbf{z})||p)} \mathbb{P}_{\mathbf{Z} \sim D^m}(\mathbf{Z} = \mathbf{z}) \\
&= \sum_{0 \leq k \leq m} e^{m \text{kl}(\frac{k}{m}||p)} \mathbb{P}_{\mathbf{Z} \sim D^m}(mq(\mathbf{Z}) = k) \\
&= \sum_{0 \leq k \leq m} \binom{m}{k} e^{m \text{kl}(\frac{k}{m}||p)} p^k (1-p)^{m-k} \\
&= \sum_{0 \leq k \leq m} \binom{m}{k} e^{m(\frac{k}{m} \ln \frac{k}{m} + (1-\frac{k}{m}) \ln(1-\frac{k}{m}))} \\
&= \sum_{0 \leq k \leq m} \binom{m}{k} \left(\frac{k}{m}\right)^k \left(1-\frac{k}{m}\right)^{m-k}.
\end{aligned}$$

However, it is obvious that, from the definition of the binomial distribution,

$$\forall m \in \mathbb{N}, \forall k \in [0, m], \forall t \in [0, 1], \binom{m}{k} t^k (1-t)^{m-k} \leq 1.$$

This is obviously the case for  $t = \frac{k}{m}$ , which gives

$$\sum_{0 \leq k \leq m} \binom{m}{k} \left(\frac{k}{m}\right)^k \left(1-\frac{k}{m}\right)^{m-k} \leq \sum_{0 \leq k \leq m} 1 = m + 1. \quad \square$$

**Theorem 6** (Jensen's inequality). *Let  $f \in \mathbb{R}^{\mathcal{X}}$  be a convex function. For all probability distribution  $P$  on  $\mathcal{X}$ :*

$$f(\mathbb{E}_{X \sim P} X) \leq \mathbb{E}_{X \sim P} f(X).$$

*Proof.* Directly comes by induction on the definition of a convex function.  $\square$

**Theorem 7** (Markov's Inequality). *Let  $X$  be a positive random variable on  $\mathbb{R}$ , such that  $\mathbb{E}X < \infty$ .*

$$\forall t \in \mathbb{R}, \mathbb{P}_X \left\{ X \geq \frac{\mathbb{E}X}{t} \right\} \leq \frac{1}{t}.$$

Consequently, if  $M \geq \mathbb{E}X$ ,

$$\forall t \in \mathbb{R}, \mathbb{P}_X \left\{ X \geq \frac{M}{t} \right\} \leq \frac{1}{t}.$$

*Proof.* Can be found on almost all textbooks on probability; see, e.g., (Devroye et al., 1997).  $\square$

**Lemma 6.**  $\forall p, q, r, s \in [0, 1], \forall \alpha \in [0, 1],$

$$\begin{aligned}
& \text{kl}(\alpha p + (1-\alpha)q || \alpha r + (1-\alpha)s) \\
& \leq \alpha \text{kl}(p||r) + (1-\alpha) \text{kl}(q||s).
\end{aligned}$$

*Proof.* It suffices to see that  $f \in \mathbb{R}^{[0,1]^2}$ ,  $f(\mathbf{v} = [p \ q]) = \text{kl}(q||p)$  is convex over  $[0, 1]^2$ : the Hessian  $H$  of  $f$  is

$$H = \begin{bmatrix} \frac{q}{p^2} + \frac{1-q}{(1-p)^2} & -\frac{1}{p} - \frac{1}{1-p} \\ -\frac{1}{p} - \frac{1}{1-p} & \frac{1}{q} + \frac{1}{1-q} \end{bmatrix},$$

and, for  $p, q \in [0, 1]$ ,  $\frac{q}{p^2} + \frac{1-q}{(1-p)^2} \geq 0$  and  $\det H = \frac{(p-q)^2}{q(1-q)p^2(1-p)^2} \geq 0$ . Hence,  $H \succeq 0$  and  $f$  is indeed convex.  $\square$

## References

- Agarwal, S., Graepel, T., Herbrich, R., Har-Peled, S., & Roth, D. (2005). Generalization bounds for the area under the roc curve. *Journal of Machine Learning Research*, 6, 393–425.
- Ambroladze, A., Parrado-Hernandez, E., & Shawe-Taylor, J. (2007). Tighter pac-bayes bounds. *Advances in Neural Information Processing Systems 19* (pp. 9–16).
- Cortes, C., & Mohri, M. (2004). AUC optimization vs. error rate minimization. *Advances in Neural Information Processing Systems 16*. MIT Press.
- Devroye, L., Györfi, L., & Lugosi, G. (1997). *A probabilistic theory of pattern recognition*. Springer.
- Janson, S. (2004). Large deviations for sums of partly dependent random variables. *Random Structures Algorithms*, 24, 234–248.
- Langford, J. (2005). Tutorial on Practical Theory for Classification. *Journal of Machine Learning Research*, 273–306.
- McAllester, D. (1999). Some pac-bayesian theorems. *Machine Learning*, 37, 355–363.
- Schreinerman, E., & Ullman, D. (1997). *Fractional graph theory: A rational approach to the theory of graphs*. Wiley Interscience Series in Discrete Mathematics.
- Seeger, M. (2002). Pac-bayesian generalization bounds for gaussian processes. *Journal of Machine Learning Research*, 3, 233–269.
- Usunier, N., Amini, M.-R., & Gallinari, P. (2006). Generalization error bounds for classifiers trained with interdependent data. *Advances in Neural Information Processing Systems 18* (pp. 1369–1376).